10/660,556

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NEWS EXPRESS	OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
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* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:10:54 ON 23 NOV 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 08:11:15 ON 23 NOV 2004
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Property values tagged with IC are from the ZIC/VINITI data file

provided by InfoChem.

STRUCTURE FILE UPDATES: 21 NOV 2004 HIGHEST RN 785750-23-4
DICTIONARY FILE UPDATES: 21 NOV 2004 HIGHEST RN 785750-23-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

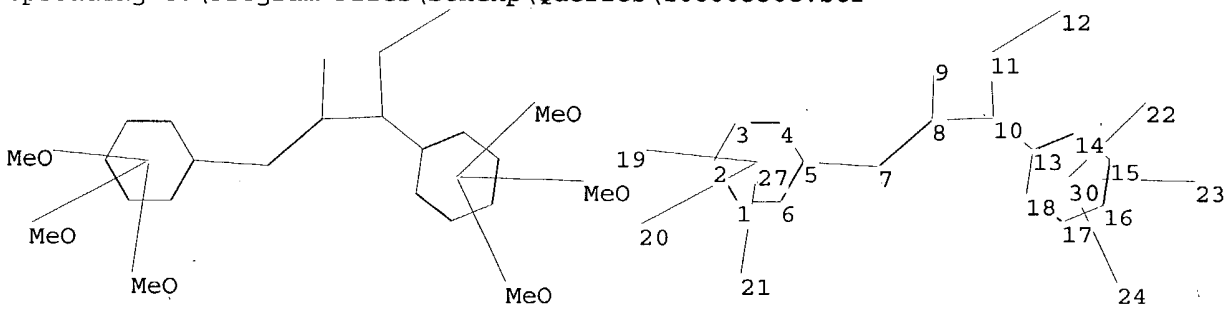
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=>
Uploading C:\Program Files\Stnexp\Queries\10660556c.str



chain nodes :
7 8 9 10 11 12 19 20 21 22 23 24
ring nodes :
1 2 3 4 5 6 13 14 15 16 17 18
chain bonds :
5-7 7-8 8-9 8-10 10-11 10-13 11-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
exact bonds :
5-7 7-8 8-9 8-10 10-11 10-13 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
isolated ring systems :
containing 1 : 13 :

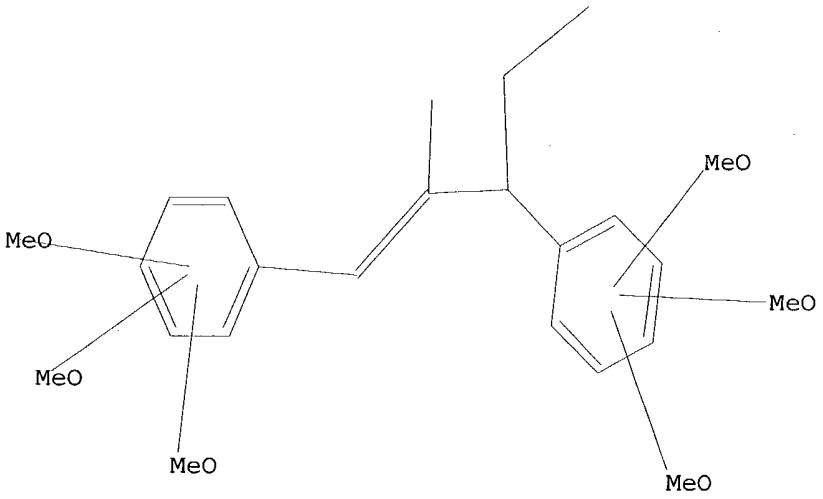
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
28:CLASS 29:CLASS 30:CLASS

L1 STRUCTURE UPLOADED

=> que L1

L2 QUE L1

=> d
L2 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.
L2 QUE L1

=> s l2
SAMPLE SEARCH INITIATED 08:11:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 140 TO ITERATE

100.0% PROCESSED 140 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2091 TO 3509
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L1

=> s l2 ful
FULL SEARCH INITIATED 08:11:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3331 TO ITERATE

100.0% PROCESSED 3331 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

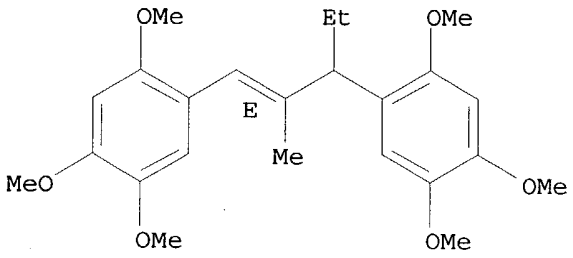
L4 2 SEA SSS FUL L1

=> d scan

L4 2 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzene, 1,1'-[(1E)-3-ethyl-2-methyl-1-propene-1,3-diyl]bis[2,4,5-

trimethoxy- (9CI)
MF C24 H32 O6

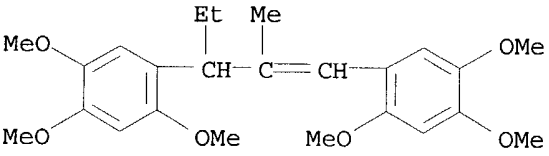
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 2 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzene, 1,1'-(3-ethyl-2-methyl-1-propene-1,3-diyl)bis[2,4,5-trimethoxy- (9CI)
MF C24 H32 O6

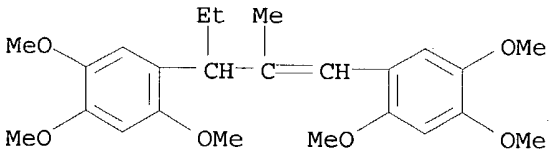


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> d 1-2

L4 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2004 ACS on STN
RN 156246-57-0 REGISTRY
CN Benzene, 1,1'-(3-ethyl-2-methyl-1-propene-1,3-diyl)bis[2,4,5-trimethoxy- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H32 O6
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PREP (Preparation)

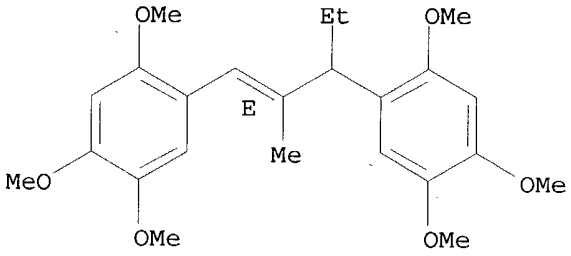


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2004 ACS on STN
RN 80423-94-5 REGISTRY
CN Benzene, 1,1'-[(1E)-3-ethyl-2-methyl-1-propene-1,3-diyl]bis[2,4,5-trimethoxy- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzene, 1,1'-(3-ethyl-2-methyl-1-propene-1,3-diyl)bis[2,4,5-trimethoxy-, (E)-
OTHER NAMES:
CN Diasarone 1
CN NEOLASA-I
FS STEREOSEARCH
DR 130766-51-7, 82373-98-6
MF C24 H32 O6
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, NAPRALERT, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file ca caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	159.80	160.01

FILE 'CA' ENTERED AT 08:13:08 ON 23 NOV 2004
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=> s l4
L5 14 L4

=> dup rem l5
PROCESSING COMPLETED FOR L5
L6 7 DUP REM L5 (7 DUPLICATES REMOVED)

=> d 1-7 bib ab

L6 ANSWER 1 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 1
AN 139:292100 CA
TI Formation of neolignan by DDQ mediated dimerization of dihydroasarone
IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi
PA Council of Scientific and Industrial Research, India
SO PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003080551	A1	20031002	WO 2002-IN73	20020327

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI WO 2002-IN73 20020327
OS CASREACT 139:292100
AB The present invention relates to a novel neolignan 3-ethyl-2-methyl-3-(2'',4'',5''-trimethoxyphenyl)-1-(2',4',5'-trimethoxyphenyl)-1-propene and a process for the preparation of high purity, high yield neolignan, α-asarone, and 2,4,5-trimethoxyphenylpropionone from β-asarone or β-asarone rich Acorus calamus oil containing α- and γ-asarone by hydrogenating and dimerizing by treatment with DDQ in presence of an organic acid.
RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 2
AN 139:292099 CA
TI DDQ-mediated one step dimerization of β-asarone or β-asarone rich Acorus calamus oil in the formation of novel neolignan
IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi
PA Council of Scientific & Industrial Research, India
SO U.S. Pat. Appl. Publ., 20 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003187306	A1	20031002	US 2002-108269	20020328
	US 2004049085	A1	20040311	US 2003-660556	20030912
PRAI	US 2002-108269	B3	20020328		

OS CASREACT 139:292099

AB The present invention relates to a novel neolignan, 3-ethyl-2-methyl-3-(2'',4'',5''-trimethoxyphenyl)-1-(2',4',5'-trimethoxyphenyl)-1-(2',4',5'-trimethoxy)phenyl-1-propene [NEOLASA-I (I)], and a process for the preparation of high purity, higher yield neolignan, α-asarone, 2,4,5-trimethoxy-phenylpropionone from β-asarone (II) or β-asarone rich Acorus calamus oil containing α- and γ-asarone by hydrogenating and dimerizing by treatment with DDQ in presence of an organic acid.

L6 ANSWER 3 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 3

AN 121:82863 CA

TI Chemical structure of 1,3-bis(2,4,5-trimethoxy)phenyl-2-methyl-pentene-1

AU Liu, Buming; Ye, Chao; Jiang, Weiheng

CS Guangxi Inst. Traditional Med. Pharm., Nanning, 530022, Peop. Rep. China

SO Fenxi Huaxue (1994), 22(4), 355-8
CODEN: FHHHDT; ISSN: 0253-3820

DT Journal

LA Chinese

AB A new compound of lignans separated from the mother liquor of recrystn. in industrial synthesis of α-asaricin was reported. The structure of the compound was determined by UV, IR, 1H-NMR, 13C-NMR and MS, and revealed to be 1,3-bis(2,4,5-trimethoxy)phenyl-2-methyl-1-pentene (I). The compound was synthesized by photochem. reaction using the above mentioned mother liquor. A possible reaction mechanism was also discussed.

L6 ANSWER 4 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 4

AN 115:278048 CA

TI Light-induced transformation of asarone

AU Lander, V.; Schreier, P.

CS Univ. Wuerzburg, Wuerzburg, D-8700, Germany

SO Flavour and Fragrance Journal (1991), 6(1), 21-8
CODEN: FFJOED; ISSN: 0882-5734

DT Journal

LA English

AB The stability of α-(I) and β-asarone (II) in ethanolic solns. was studied under daylight conditions over a period of 6 mo. After rapid initial light-induced isomerization of I to II, a number of oxidation products, i.e. 2,4,5-trimethoxybenzaldehyde, 1-(2,4,5-trimethoxyphenyl) propan-2-one, and 2,4,5-trimethoxypropiophenone and addition products, i.e. 1-ethoxy-1-(2,4,5-trimethoxyphenyl)propane, (1R,2R; 1S,2S)-1-ethoxy-1-(2,4,5-trimethoxyphenyl)propan-2-ol, (1R,2S; 1S,2R)-1-ethoxy-1-(2,4,5-trimethoxyphenylpropan-2-ol, (1R,2R; 1S,2S)-1-(2,4,5-trimethoxyphenyl)propan-1,2-diol, and (1R,2S; 1S,2R)-1-(2,4,5-trimethoxyphenyl)propan-1,2-diol, as well as the dimers 1-(2',4',5'-trimethoxyphenyl)-2-methyl-3-(2,4,5-trimethoxyphenyl)-1E-pentene (III) and 1-(2',4',5'-trimethoxyphenyl)-2-methyl-3-ethyl-1α,2β,3α(II)-4,6,7-trimethoxyindane (IV) were detected after extractive sample preparation In addition, 3 dimers, 1-(2',4',5'-trimethoxyphenyl)-2-methyl-3(2,4,5-trimethoxyphenyl)-penta-1E,4-diene, 1-(2',4',5'-trimethoxyphenyl)-2-(2,4,5-trimethoxyphenyl)-3,4-dimethylcyclobutane, and 1-(2',4',5'-trimethoxyphenyl)-2-methyl-3-(2,4,5-trimethoxyphenyl)prop-1-en-3-one were tentatively identified. Identification was carried out by capillary gas chromatog. (HRGC) and online HRGC techniques, i.e. HRGC mass spectrometry and HRGC-Fourier transform IR spectroscopy as well as 1H-NMR spectroscopy.

L6 ANSWER 5 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 5
AN 113:241942 CA
TI Structure of (E)-2-methyl-1,3-bis(2,4,5-trimethoxyphenyl)-1-pentene and 1-(2,4,5-trimethoxyphenyl)-2-methyl-3-ethyl-4,6,7-trimethoxyindan C24H32O6: two asarone dimers
AU Lemini, C.; Mandoki, J. J.; Cruz-Almanza, R.; Toscano, R. A.
CS Fac. Med., UNAM, Coyoacan, 04510, Mex.
SO Acta Crystallographica, Section C: Crystal Structure Communications (1990), C46(8), 1542-5
CODEN: ACSCEE; ISSN: 0108-2701
DT Journal
LA English
AB (E)-2-Methyl-1,3-bis(2,4,5-trimethoxyphenyl)-1-pentene (I) is monoclinic, space group P21/n, with a 7.082(3), b 11.954(7), c 27.136(17) Å, and β 94.14(4)°; d.(calculated) = 1.21 for Z = 4. Final R = 0.056 and Rw = 0.063 for 2901 reflections. 1-(2,4,5-Trimethoxyphenyl)-2-methyl-3-ethyl-4,6,7-trimethoxyindan (II) is monoclinic space group P21/a with a 17.281(5), b 7.701(1), c 18.057(6) Å, and β 108.23(2)°; d.(calculated) = 1.21 for Z = 4. Final R = 0.045 and Rw = 0.061 for 2601 reflections. Atomic coordinates are given. The x-ray structures confirm the structures previously assigned on the basis of chemical and NMR spectral evidence. I is non-planar. In II the 5-membered ring adopts an envelope conformation and the substituents at C(1) and C(3) are antiperiplanar to the Me group at C(2). In both isomers the orientation of the trimethoxyphenyl substituent is determined by C-H...O intramol. interactions. The packing in the crystal is entirely due to van der Waals forces.

L6 ANSWER 6 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 6
AN 97:38740 CA
TI The active substances of Asarum europeum L. XV. Structure of the diasarones
AU Bohlmann, Ferdinand; Gracza, Lajos
CS Inst. Org. Chem., Tech. Univ. Berlin, Berlin, D 1000, Fed. Rep. Ger.
SO Archiv der Pharmazie (Weinheim, Germany) (1982), 315(5), 474-6 RS1,A7
CODEN: ARPMAS; ISSN: 0365-6233
DT Journal
LA German
AB Diasarone, prepared by the method of T. Szeki (1906), consists of 2 substances, diasarone-1 (I) and diasarone-2 (II).

L6 ANSWER 7 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 7
AN 96:34762 CA
TI Synthesis of a novel asarone dimer
AU Lemini, C.; Cruz, R.; Sanchez, I. H.
CS Fac. Med., Univ. Nac. Auton. Mexico, Mexico City, Mex.
SO Organic Preparations and Procedures International (1981), 13(5), 374-8
CODEN: OPPIAK; ISSN: 0030-4948
DT Journal
LA English
AB Title compds. I and II were prepared as anticholesteremics (no data). Thus, asarone was treated at room temperature with PBr3 for 3 h to give 87% E-I. Treating I with PBr3 for 24 h gave 78% II. I was converted to II by acid catalysis.

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	20.80	180.81

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL

10/660,556

	ENTRY	SESSION
CA SUBSCRIBER PRICE	-4.62	-4.62

STN INTERNATIONAL LOGOFF AT 08:18:04 ON 23 NOV 2004